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A simple diatomic potential that prevents crystallization in supercooled liquids simulations

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Titre	A simple diatomic potential that prevents crystallization in supercooled liquids simulations
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Auteur	Kerasidou, Ariadni P. [1], Mauboussin, Yannick [2], Teboul, Victor [3]
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Type	Article scientifique dans une revue à comité de lecture
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Résumé en anglais	We study a simple and versatile diatomic potential function coined to prevent crystallization in supercooled liquids. We show that the corresponding liquid doesn't crystallize even with very long simulation runs at the lowest temperature that we can access with ergodic simulations. The medium displays the usual features of supercooled materials and a non-Arrhenius dependence of the diffusion coefficient and α relaxation time with temperature. We also observe the breakdown of the Stokes-Einstein relation at low temperatures.
URL de la notice	http://okina.univ-angers.fr/publications/ua8566 [4]
DOI	10.1016/j.chemphys.2015.02.009 [5]

Liens

[1] http://okina.univ-angers.fr/akerasi/publications
[2] http://okina.univ-angers.fr/publications?f[author]=1805
[3] http://okina.univ-angers.fr/v.teboul/publications
[4] http://okina.univ-angers.fr/publications/ua8566
[5] http://dx.doi.org/10.1016/j.chemphys.2015.02.009

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